Glenn T. Seaborg Center Seminar

Recent Progress in Computational Modeling of Actinide Complexes

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4:00 - 5:00 pm
Building 70A, Room 3377

Actinide compounds are challenging to computational chemistry because of the complicated electron correlation effects and relativistic effects. There have been significant developments in theoretical studies on actinide compounds in the past several years. In this talk, we will provide an overview of our own research in this field, with particular emphasis on applications of relativistic quantum chemical methods to the electronic structures of small actinide molecules and some large actinide compounds relevant to separation and environment science. The performance of various density functional approaches and wavefunction-based electron correlation methods will be compared. The results of computational modeling on the vibrational, electronic, and NMR spectra of actinide compounds will also be discussed.

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